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2-(2,4-Dichlorophenyl)-3-[5-(3,5-dimethylphenyl)-1,3,4-thiadiazol-2-yl]-thiazolidin-4-one

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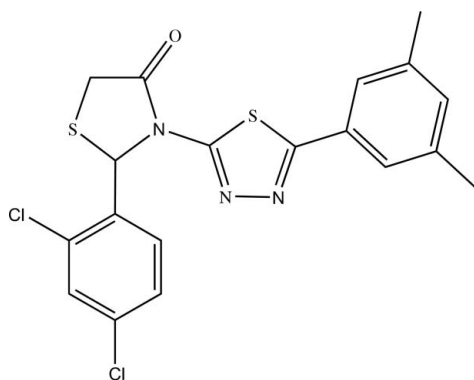
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å; R factor = 0.055; wR factor = 0.165; data-to-parameter ratio = 15.4.

The title compound, $\text{C}_{19}\text{H}_{15}\text{Cl}_2\text{N}_3\text{OS}_2$, was synthesized by the reaction of *N*-(2,4-dichlorophenyl)-5-(3,5-dimethylphenyl)-1,3,4-thiadiazol-2-amine and mercaptoacetic acid. The thiazolidinone ring adopts a twist conformation. The 2,4-dichlorophenyl ring is almost perpendicular to the thiaziazole ring, the dihedral angle being $82.8(2)^\circ$. The 3,5-dimethylphenyl ring is nearly coplanar with the thiaziazole ring, the dihedral angle being $2.7(2)^\circ$. An intramolecular $\text{C}-\text{H}\cdots\text{N}$ hydrogen bond is present.

Related literature

For general background, see: Arun *et al.* (1999); Chen *et al.* (2000); Kidwai *et al.* (2000); Vicentini *et al.* (1998); Wasfy *et al.* (1996). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$\text{C}_{19}\text{H}_{15}\text{Cl}_2\text{N}_3\text{OS}_2$
 $M_r = 436.36$
Triclinic, $P\bar{1}$

$a = 8.1760(16)$ Å
 $b = 9.1650(18)$ Å
 $c = 14.483(3)$ Å

$\alpha = 80.60(3)^\circ$
 $\beta = 80.82(3)^\circ$
 $\gamma = 63.92(3)^\circ$
 $V = 956.9(4)$ Å³
 $Z = 2$

Mo $K\alpha$ radiation
 $\mu = 0.57$ mm⁻¹
 $T = 298(2)$ K
 $0.40 \times 0.30 \times 0.20$ mm

Data collection

Enraf-Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
 $T_{\min} = 0.803$, $T_{\max} = 0.894$
4042 measured reflections

3761 independent reflections
2824 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.044$
3 standard reflections every 200 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.055$
 $wR(F^2) = 0.165$
 $S = 1.03$
3761 reflections

244 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 0.42$ e Å⁻³
 $\Delta\rho_{\min} = -0.45$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C15}-\text{H15A}\cdots\text{N3}$	0.93	2.49	2.842 (6)	102

Data collection: *CAD-4 Software* (Enraf-Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXL97*.

The authors thank Professor Hua-qin Wang of Nanjing University for carrying out the X-ray crystallographic analysis.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RN2029).

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supporting information

Acta Cryst. (2008). E64, o260 [https://doi.org/10.1107/S1600536807066068]

2-(2,4-Dichlorophenyl)-3-[5-(3,5-dimethylphenyl)-1,3,4-thiadiazol-2-yl]thiazolidin-4-one

Rong Wan, Li-he Yin, Feng Han, Bin Wang and Jin-tang Wang

S1. Comment

1,3,4-Thiadiazole derivatives containing the thiazolidinone unit are of great interest because of their chemical and pharmaceutical properties. Some derivatives have fungicidal activities and exhibit certain herbicidal activities (Chen *et al.*, 2000; Kidwai *et al.*, 2000; Vicentini *et al.*, 1998). Some show insecticidal activities (Arun *et al.*, 1999; Wasfy *et al.*, 1996). We report here the crystal structure of the titled compound, (I).

The molecular structure of (I) is shown in Fig.1. In this structure, the thiazolidinone adopts a twist conformation, the dihedral angle between the C11/S1/C12 and C11/N3/C12 is 24.4 (4)°. The thiadiazole ring (S2/C9/N1/N2/C10) is an aromatic heterocyclic ring, all atoms are in the same plane. The angle between the thiadiazole ring and the 3,5-dimethylphenyl ring is 2.7 (2)°. The other benzene ring (C14/C15/C16/C17/C18/C19) is nearly perpendicular to the thiadiazole ring, the dihedral angle is 82.8 (2)°. The molecule has a C—H···N intramolecular hydrogen bond.

S2. Experimental

N-(2,4-dichlorobenzylidene)-5-(3,5-dimethylphenyl)-1,3,4-thiadiazol-2-amine (5 mmol) and mercapto-acetic acid (5 mmol) were added in toluene (50 ml). The water was removed by distillation for 5 h. The reaction mixture was left to cool to room temperature, filtered, and the filter cake was crystallized from acetone to give pure compound (I) (m.p. 476–477 K). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an acetone solution.

S3. Refinement

All H atoms bonded to the C atoms were placed geometrically at the distances of 0.93–0.97 Å and constrained to ride on their parent atoms with $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C})$, where $x = 1.2$ for aromatic H and $x = 1.5$ for methyl H atoms. The methyl groups were allowed to rotate.

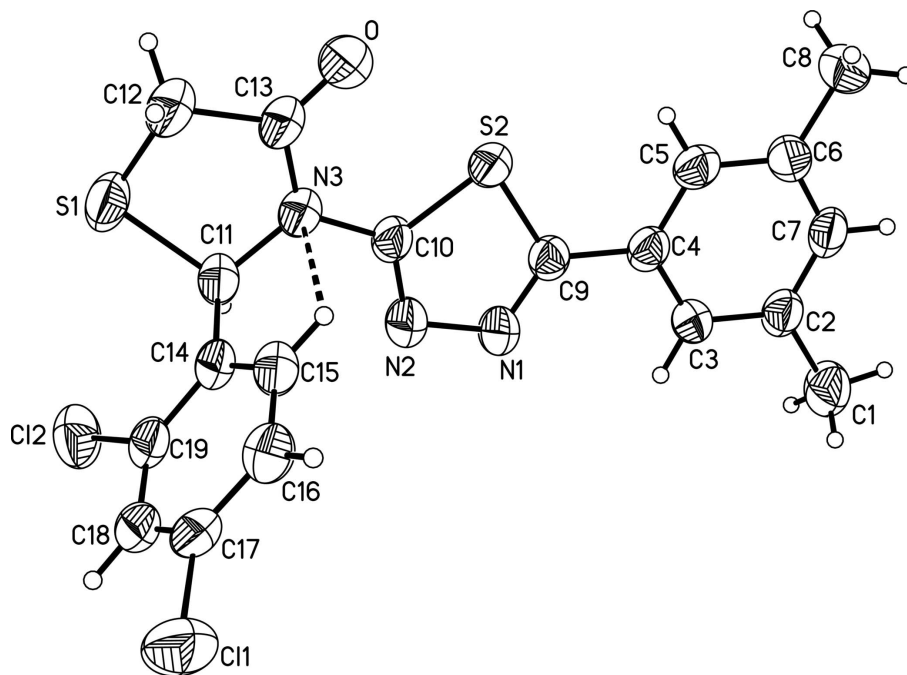


Figure 1

The crystal structure of (I). Dashed lines indicate intramolecular C—H...N hydrogen bond.

2-(2,4-Dichlorophenyl)-3-[5-(3,5-dimethylphenyl)-1,3,4-thiadiazol-2-yl]thiazolidin-4-one

Crystal data

$C_{19}H_{15}Cl_2N_3OS_2$

$M_r = 436.36$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 8.1760$ (16) Å

$b = 9.1650$ (18) Å

$c = 14.483$ (3) Å

$\alpha = 80.60$ (3)°

$\beta = 80.82$ (3)°

$\gamma = 63.92$ (3)°

$V = 956.9$ (4) Å³

$Z = 2$

$F(000) = 448$

$D_x = 1.514$ Mg m⁻³

Melting point = 476–477 K

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 25 reflections

$\theta = 10$ – 14°

$\mu = 0.57$ mm⁻¹

$T = 298$ K

Block, light yellow

$0.40 \times 0.30 \times 0.20$ mm

Data collection

Enraf–Nonius CAD-4

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\omega/2\theta$ scans

Absorption correction: ψ scan

(North *et al.*, 1968)

$T_{\min} = 0.803$, $T_{\max} = 0.894$

4042 measured reflections

3761 independent reflections

2824 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.044$

$\theta_{\max} = 26.0^\circ$, $\theta_{\min} = 1.4^\circ$

$h = -9 \rightarrow 10$

$k = -11 \rightarrow 11$

$l = 0 \rightarrow 17$

3 standard reflections every 200 reflections

intensity decay: none

*Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.055$ $wR(F^2) = 0.165$ $S = 1.04$

3761 reflections

244 parameters

0 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 2.5P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 0.42 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.45 \text{ e } \text{\AA}^{-3}$ *Special details*

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	0.6127 (2)	0.7754 (2)	-0.14356 (11)	0.0843 (5)
Cl2	1.25961 (17)	0.62298 (16)	-0.02409 (9)	0.0667 (4)
S1	1.13265 (18)	0.90179 (17)	0.12924 (9)	0.0626 (4)
S2	0.80372 (16)	0.67126 (13)	0.42066 (7)	0.0469 (3)
O	0.7989 (6)	0.9660 (4)	0.3520 (3)	0.0818 (12)
N1	0.9137 (5)	0.4033 (4)	0.3485 (2)	0.0522 (9)
N2	0.9641 (5)	0.5066 (4)	0.2796 (2)	0.0523 (9)
N3	0.9527 (5)	0.7697 (4)	0.2528 (2)	0.0487 (8)
C1	0.7096 (8)	-0.0041 (6)	0.5859 (4)	0.0672 (13)
H1B	0.6622	-0.0377	0.6465	0.101*
H1C	0.8348	-0.0796	0.5727	0.101*
H1D	0.6386	-0.0023	0.5386	0.101*
C2	0.6989 (6)	0.1640 (6)	0.5861 (3)	0.0514 (11)
C3	0.7698 (6)	0.2378 (5)	0.5073 (3)	0.0469 (10)
H3A	0.8261	0.1815	0.4547	0.056*
C4	0.7565 (6)	0.3936 (5)	0.5074 (3)	0.0439 (9)
C5	0.6693 (6)	0.4783 (6)	0.5844 (3)	0.0496 (10)
H5A	0.6602	0.5831	0.5842	0.059*
C6	0.5944 (6)	0.4091 (6)	0.6629 (3)	0.0486 (10)
C7	0.6134 (6)	0.2527 (6)	0.6616 (3)	0.0527 (11)
H7A	0.5664	0.2048	0.7140	0.063*
C8	0.4899 (7)	0.5073 (7)	0.7442 (3)	0.0698 (14)
H8A	0.4485	0.4418	0.7920	0.105*
H8B	0.3863	0.6025	0.7226	0.105*
H8C	0.5683	0.5402	0.7698	0.105*

C9	0.8307 (5)	0.4717 (5)	0.4236 (3)	0.0409 (9)
C10	0.9149 (6)	0.6481 (5)	0.3094 (3)	0.0443 (9)
C11	1.0540 (6)	0.7385 (5)	0.1604 (3)	0.0480 (10)
H11A	1.1602	0.6323	0.1651	0.058*
C12	0.9563 (9)	1.0308 (7)	0.2078 (4)	0.0745 (16)
H12A	1.0026	1.0901	0.2380	0.089*
H12B	0.8546	1.1093	0.1738	0.089*
C13	0.8942 (7)	0.9217 (6)	0.2809 (3)	0.0576 (12)
C14	0.9401 (6)	0.7419 (5)	0.0871 (3)	0.0431 (9)
C15	0.7515 (6)	0.7987 (5)	0.1026 (3)	0.0500 (10)
H15A	0.6923	0.8314	0.1610	0.060*
C16	0.6505 (6)	0.8074 (6)	0.0324 (3)	0.0532 (11)
H16A	0.5239	0.8462	0.0431	0.064*
C17	0.7404 (7)	0.7576 (5)	-0.0542 (3)	0.0538 (11)
C18	0.9264 (6)	0.6968 (5)	-0.0713 (3)	0.0505 (10)
H18A	0.9855	0.6604	-0.1290	0.061*
C19	1.0239 (6)	0.6911 (5)	-0.0003 (3)	0.0461 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.1062 (12)	0.1000 (11)	0.0749 (9)	-0.0627 (10)	-0.0278 (8)	-0.0105 (8)
C12	0.0586 (7)	0.0700 (8)	0.0645 (8)	-0.0285 (6)	0.0135 (6)	-0.0046 (6)
S1	0.0718 (8)	0.0738 (8)	0.0616 (7)	-0.0531 (7)	-0.0053 (6)	0.0051 (6)
S2	0.0603 (7)	0.0507 (6)	0.0407 (5)	-0.0345 (5)	-0.0035 (5)	-0.0034 (4)
O	0.130 (3)	0.067 (2)	0.062 (2)	-0.061 (2)	0.020 (2)	-0.0169 (18)
N1	0.071 (2)	0.051 (2)	0.0410 (19)	-0.0354 (19)	0.0016 (17)	0.0019 (16)
N2	0.064 (2)	0.050 (2)	0.046 (2)	-0.0316 (18)	0.0043 (17)	-0.0019 (16)
N3	0.060 (2)	0.049 (2)	0.0456 (19)	-0.0339 (18)	-0.0029 (16)	-0.0006 (16)
C1	0.079 (3)	0.058 (3)	0.066 (3)	-0.037 (3)	0.006 (3)	0.000 (2)
C2	0.063 (3)	0.065 (3)	0.041 (2)	-0.042 (2)	-0.007 (2)	0.003 (2)
C3	0.056 (2)	0.055 (2)	0.037 (2)	-0.032 (2)	0.0002 (18)	-0.0044 (18)
C4	0.048 (2)	0.053 (2)	0.041 (2)	-0.0301 (19)	-0.0090 (17)	0.0004 (18)
C5	0.057 (3)	0.059 (3)	0.047 (2)	-0.035 (2)	-0.0089 (19)	-0.006 (2)
C6	0.046 (2)	0.070 (3)	0.039 (2)	-0.032 (2)	-0.0046 (17)	-0.009 (2)
C7	0.061 (3)	0.078 (3)	0.038 (2)	-0.049 (2)	-0.0068 (19)	0.005 (2)
C8	0.075 (3)	0.095 (4)	0.056 (3)	-0.049 (3)	0.009 (2)	-0.028 (3)
C9	0.039 (2)	0.048 (2)	0.040 (2)	-0.0232 (18)	-0.0042 (16)	-0.0029 (17)
C10	0.058 (2)	0.052 (2)	0.034 (2)	-0.035 (2)	-0.0088 (17)	0.0044 (17)
C11	0.053 (2)	0.053 (2)	0.043 (2)	-0.031 (2)	0.0003 (18)	0.0011 (18)
C12	0.114 (5)	0.069 (3)	0.062 (3)	-0.064 (3)	-0.001 (3)	0.002 (3)
C13	0.080 (3)	0.052 (3)	0.053 (3)	-0.043 (2)	-0.001 (2)	0.000 (2)
C14	0.051 (2)	0.040 (2)	0.042 (2)	-0.0264 (18)	-0.0002 (18)	0.0020 (17)
C15	0.056 (3)	0.059 (3)	0.043 (2)	-0.035 (2)	-0.0004 (19)	-0.0006 (19)
C16	0.046 (2)	0.058 (3)	0.059 (3)	-0.027 (2)	-0.002 (2)	-0.004 (2)
C17	0.075 (3)	0.052 (3)	0.053 (3)	-0.043 (2)	-0.007 (2)	-0.004 (2)
C18	0.071 (3)	0.040 (2)	0.048 (2)	-0.033 (2)	0.005 (2)	-0.0052 (18)
C19	0.055 (2)	0.040 (2)	0.047 (2)	-0.0287 (19)	0.0016 (19)	0.0013 (17)

Geometric parameters (Å, °)

C11—C17	1.734 (5)	C5—C6	1.398 (6)
C12—C19	1.739 (4)	C5—H5A	0.9300
S1—C12	1.786 (6)	C6—C7	1.375 (6)
S1—C11	1.841 (4)	C6—C8	1.509 (6)
S2—C10	1.716 (4)	C7—H7A	0.9300
S2—C9	1.738 (4)	C8—H8A	0.9600
O—C13	1.198 (6)	C8—H8B	0.9600
N1—C9	1.285 (5)	C8—H8C	0.9600
N1—N2	1.401 (5)	C11—C14	1.507 (6)
N2—C10	1.303 (5)	C11—H11A	0.9800
N3—C13	1.368 (6)	C12—C13	1.518 (6)
N3—C10	1.391 (5)	C12—H12A	0.9700
N3—C11	1.458 (5)	C12—H12B	0.9700
C1—C2	1.504 (6)	C14—C15	1.386 (6)
C1—H1B	0.9600	C14—C19	1.388 (6)
C1—H1C	0.9600	C15—C16	1.380 (6)
C1—H1D	0.9600	C15—H15A	0.9300
C2—C7	1.376 (6)	C16—C17	1.385 (6)
C2—C3	1.406 (6)	C16—H16A	0.9300
C3—C4	1.383 (6)	C17—C18	1.365 (6)
C3—H3A	0.9300	C18—C19	1.378 (6)
C4—C5	1.378 (6)	C18—H18A	0.9300
C4—C9	1.488 (5)		
C12—S1—C11	92.2 (2)	N1—C9—S2	114.6 (3)
C10—S2—C9	86.20 (19)	C4—C9—S2	120.6 (3)
C9—N1—N2	112.7 (3)	N2—C10—N3	120.8 (4)
C10—N2—N1	110.8 (3)	N2—C10—S2	115.7 (3)
C13—N3—C10	121.6 (4)	N3—C10—S2	123.5 (3)
C13—N3—C11	118.1 (3)	N3—C11—C14	113.4 (3)
C10—N3—C11	120.2 (3)	N3—C11—S1	104.4 (3)
C2—C1—H1B	109.5	C14—C11—S1	110.7 (3)
C2—C1—H1C	109.5	N3—C11—H11A	109.4
H1B—C1—H1C	109.5	C14—C11—H11A	109.4
C2—C1—H1D	109.5	S1—C11—H11A	109.4
H1B—C1—H1D	109.5	C13—C12—S1	107.3 (4)
H1C—C1—H1D	109.5	C13—C12—H12A	110.3
C7—C2—C3	117.9 (4)	S1—C12—H12A	110.3
C7—C2—C1	121.2 (4)	C13—C12—H12B	110.3
C3—C2—C1	120.9 (4)	S1—C12—H12B	110.3
C4—C3—C2	120.5 (4)	H12A—C12—H12B	108.5
C4—C3—H3A	119.8	O—C13—N3	124.4 (4)
C2—C3—H3A	119.8	O—C13—C12	124.1 (4)
C5—C4—C3	119.7 (4)	N3—C13—C12	111.5 (4)
C5—C4—C9	120.0 (4)	C15—C14—C19	117.8 (4)
C3—C4—C9	120.3 (4)	C15—C14—C11	122.4 (4)

C4—C5—C6	121.0 (4)	C19—C14—C11	119.7 (4)
C4—C5—H5A	119.5	C16—C15—C14	120.9 (4)
C6—C5—H5A	119.5	C16—C15—H15A	119.6
C7—C6—C5	117.9 (4)	C14—C15—H15A	119.6
C7—C6—C8	121.8 (4)	C15—C16—C17	119.0 (4)
C5—C6—C8	120.2 (4)	C15—C16—H16A	120.5
C6—C7—C2	123.0 (4)	C17—C16—H16A	120.5
C6—C7—H7A	118.5	C18—C17—C16	121.8 (4)
C2—C7—H7A	118.5	C18—C17—C11	119.2 (4)
C6—C8—H8A	109.5	C16—C17—C11	119.0 (4)
C6—C8—H8B	109.5	C17—C18—C19	118.0 (4)
H8A—C8—H8B	109.5	C17—C18—H18A	121.0
C6—C8—H8C	109.5	C19—C18—H18A	121.0
H8A—C8—H8C	109.5	C18—C19—C14	122.4 (4)
H8B—C8—H8C	109.5	C18—C19—C12	117.9 (3)
N1—C9—C4	124.8 (4)	C14—C19—C12	119.6 (3)
C9—N1—N2—C10	0.5 (5)	C10—N3—C11—C14	76.7 (5)
C7—C2—C3—C4	1.3 (6)	C13—N3—C11—S1	18.4 (5)
C1—C2—C3—C4	178.9 (4)	C10—N3—C11—S1	-162.7 (3)
C2—C3—C4—C5	-1.5 (6)	C12—S1—C11—N3	-22.7 (3)
C2—C3—C4—C9	-179.6 (4)	C12—S1—C11—C14	99.6 (3)
C3—C4—C5—C6	0.2 (6)	C11—S1—C12—C13	22.1 (4)
C9—C4—C5—C6	178.4 (4)	C10—N3—C13—O	-4.5 (8)
C4—C5—C6—C7	1.2 (6)	C11—N3—C13—O	174.4 (5)
C4—C5—C6—C8	-176.4 (4)	C10—N3—C13—C12	178.8 (4)
C5—C6—C7—C2	-1.4 (7)	C11—N3—C13—C12	-2.4 (6)
C8—C6—C7—C2	176.2 (4)	S1—C12—C13—O	167.6 (5)
C3—C2—C7—C6	0.2 (7)	S1—C12—C13—N3	-15.6 (6)
C1—C2—C7—C6	-177.4 (4)	N3—C11—C14—C15	11.2 (6)
N2—N1—C9—C4	178.1 (4)	S1—C11—C14—C15	-105.7 (4)
N2—N1—C9—S2	-0.3 (5)	N3—C11—C14—C19	-170.7 (3)
C5—C4—C9—N1	-179.9 (4)	S1—C11—C14—C19	72.4 (4)
C3—C4—C9—N1	-1.8 (6)	C19—C14—C15—C16	-1.3 (6)
C5—C4—C9—S2	-1.6 (5)	C11—C14—C15—C16	176.9 (4)
C3—C4—C9—S2	176.5 (3)	C14—C15—C16—C17	0.3 (7)
C10—S2—C9—N1	0.0 (3)	C15—C16—C17—C18	1.4 (7)
C10—S2—C9—C4	-178.5 (3)	C15—C16—C17—C11	-177.7 (3)
N1—N2—C10—N3	179.3 (4)	C16—C17—C18—C19	-2.1 (6)
N1—N2—C10—S2	-0.5 (5)	C11—C17—C18—C19	177.1 (3)
C13—N3—C10—N2	176.7 (4)	C17—C18—C19—C14	1.1 (6)
C11—N3—C10—N2	-2.2 (6)	C17—C18—C19—C12	-176.9 (3)
C13—N3—C10—S2	-3.5 (6)	C15—C14—C19—C18	0.6 (6)
C11—N3—C10—S2	177.7 (3)	C11—C14—C19—C18	-177.6 (4)
C9—S2—C10—N2	0.3 (3)	C15—C14—C19—C12	178.6 (3)
C9—S2—C10—N3	-179.6 (4)	C11—C14—C19—C12	0.4 (5)
C13—N3—C11—C14	-102.2 (4)		

Hydrogen-bond geometry (Å, °)

<i>D—H···A</i>	<i>D—H</i>	<i>H···A</i>	<i>D···A</i>	<i>D—H···A</i>
C15—H15A···N3	0.93	2.49	2.842 (6)	102
